

Positronium Ions and Molecules

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ABSTRACT

Recent theoretical studies on positronium ions and molecules will be discussed. A positronium ion is a three-particle system consisting of two electrons in singlet spin state, and a positron. Recent studies include calculations of its binding energy, positron annihilation rate, and investigations of its doubly excited resonant states. A positronium molecule is a four-body system consisting of two positrons and two electrons in an overall singlet spin state. We will discuss the recent calculations of its binding energy against the dissociation into two positronium atoms, and studies of auto-detaching states in positronium molecules. These auto-dissociating states, which are believed to be part of the Rydberg series as a result of a positron attaching to a negatively charged positronium ion, Ps^- , would appear as resonances in Ps - Ps scattering.

POSITRONIUM IONS

In this talk I will describe two atomic systems involving positrons. They are positronium ions and molecules. For Ps^- , I will concentrate the discussions on the recent theoretical calculations of binding energy, annihilation rate, and autoionizing resonant states. In positronium molecules, I will discuss calculations of the ground state energy and the studies of auto-dissociating states.

A positronium negative ion (Ps^-) is a bound three-particle system consisting of two electrons and one positron which interact via Coulomb forces. The calculation of the binding energy of this system has a long history that can be traced back to the early work of Wheeler.¹ This system was observed for the first time in the laboratory by Mills.² Later he also measured³ the positron annihilation rate for Ps^- . The production of these positronium negative ions have stimulated intense theoretical investigations. In the last decade, several progress reports and review articles on Ps^- have appeared in the literature.⁴⁻⁷ So here I will discuss mostly the recent advances since publication of these reviews. In many aspects the positronium negative ions have properties similar to those of hydrogen negative ions, H^- , a system which has been intensively studied by both theorists and experimentalists. Recently, the muonium ions, Mu^- , have also been observed.⁸ These three systems differ in the mass of the positively charged particles. There are, however, many properties which are unique in Ps^- and have no counterparts in H^- and Mu^- . These properties involve the annihilation of the positrons in the positronium negative ions. On the practical side, the role that the positronium negative ions play in astrophysics and space physics has been suggested by Sivaram and Krishan.⁹

Let me first talk about the calculations of ground state energy for Ps^- and its annihilation rate. For a highly correlated atomic system such as Ps^- , it is essential for the wave functions to have accurate representation of the correlation effects. There are two types of wave functions used in recent years that are proven to be quite effective to describe Ps^- . One type is of the Hylleraas wave functions, as used by Bhatia and Drachman¹⁰ (with two non-linear parameters),

and by Ho (with one non-linear parameter),¹¹

$$\Psi = \sum_{k,\ell,m \geq 0} C_{k\ell m} \exp\{-\alpha_1 r_{1p} - \alpha_2 r_{2p}\} r_{12}^k (r_{1p}^\ell r_{2p}^m + r_{1p}^m r_{2p}^\ell) . \quad (1)$$

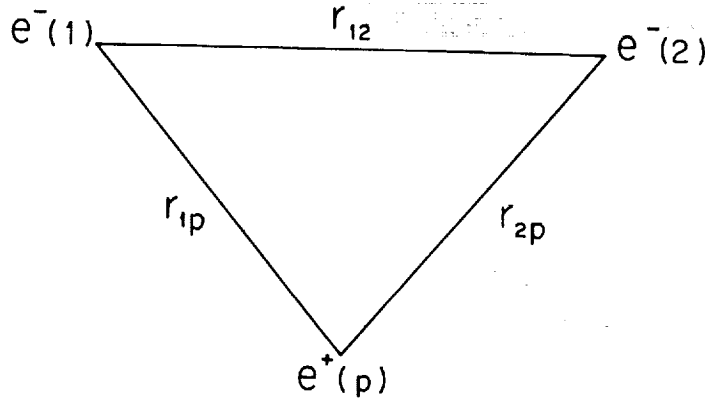


Fig. 1. Coordinate System for Ps^- .

The coordinate system is shown here in Fig. 1. The other type is the exponential variational expansion for the basis set with the form, as used by Petelenz and Smith,¹² and by Frolov and Yermi¹³,

$$\Psi = \frac{1}{\sqrt{2}}(1 + P_{12}) \sum_{i=1}^N C_i \exp(-\alpha_1^{(i)} r_{2p} - \alpha_2^{(i)} r_{1p} - \alpha_3^{(i)} r_{12}) , \quad (2)$$

where P_{12} is the permutation operator for electrons 1 and 2. C_i are linear combination coefficients, and $\alpha_j^{(i)}$ ($j = 1, 2, 3$) were generated in a quasirandomly form from three intervals. Results calculated by using these functions are shown here in Table 1. The Ho (1989)¹⁴ result is the extension of the Ho (1983) calculation with the basis set now extended to $N = 715$ terms ($\omega = k + \ell + m \leq 18$).

One of the experimentally interesting parameters is the annihilation rate, Γ , given in units of $n s^{-1}$

$$\Gamma = 2\pi\alpha^4\left(\frac{c}{a_0}\right)\left[1 - \alpha\left(\frac{17}{\pi} - \frac{19\pi}{12}\right)\right] \frac{\langle \Psi | \delta(r_e - r_p) | \Psi \rangle}{\langle \Psi | \Psi \rangle} = 100.617 \langle \delta_{ep} \rangle . \quad (3)$$

Table 1. Ground state energy of Ps^- (in Ry).

| | |
|---|---|
| Ho (1983), Ref. 11 (125 term Hylleraas function, one non-linear parameter) | -0.524009790 |
| Bhatia and Drachman (1983), Ref. 10 (220 term Hylleraas function, two non-linear parameters) | -0.5240101300 |
| Frolov (1987), Ref. 14 | -0.5240101404 |
| Petelenz and Smith (1988), Ref. 12 (150 term exponential variational expansion) | -0.524010140 |
| Ho (1989), Ref. 15 (715 term Hylleraas function) | -0.524010140 |
| Frolov and Yeremin (1989), Ref. 13 (700 term exponential variation expansion) | -0.5240101404656 $\pm 1 \times 10^{-12}$ |

The lifetime of Ps^- against annihilation is

$$\tau = \frac{1}{\Gamma}. \quad (4)$$

In Eq. (3), the correction term proportional to α is due to the triplet lifetime¹⁶ and the leading radiative correction to the singlet lifetime.¹⁷ Once the energy-minimized wavefunctions are obtained, they can be used to calculate Γ by the use of equation (3). Some recent results are shown in Table 2. It is seen that they are compared quite well with the experimental measurement of $\Gamma = 2.09 \pm 0.09 ns^{-1}$ (Ref. 3). Furthermore, some progress for an improved measurement of the annihilation rate has recently been made.¹⁸ This would stimulate further theoretical studies.

Table 2. Positron annihilation rate in Ps^- .

| | Γ (nsec ⁻¹) | ν_{ep} | Ref. |
|---|--------------------------------|------------|------|
| Bhatia and Drachman 1983 (220 term Hylleraas function) | 2.0861 | 0.50000 | 10 |
| Ho 1983 (125 term Hylleraas function) | 2.0850 | 0.4991 | 11 |
| Ho 1989 (715 term Hylleraas function) | 2.08613 | 0.50001 | 15 |
| Mills (1983) experiment | 2.09 ± 0.09 | | 3 |

The qualities of the wavefunctions can be tested by calculating the electron-electron and electron-positron cusp values. For a system interacting through Coulomb forces, the average value of the cusp condition between particles i and j is given by¹⁹

$$\nu_{ij} = \langle \Psi | \delta(r_{ij}) \frac{\partial}{\partial r_{ij}} | \Psi \rangle (\langle \Psi | \delta(r_{ij}) | \Psi \rangle)^{-1}, \quad (5)$$

and the exact value for ν_{ij} is

$$\nu_{ij} = q_i q_j \mu_{ij}, \quad (6)$$

where q_i is the charge for the particle i and μ_{ij} is the reduced mass for particles i and j . The exact values for electron-electron and electron-positron conditions are hence +0.5 and -0.5 respectively. The positron-electron cusp values calculated in the recent calculations are also shown here in Table 2. It is seen that the cusp results are very close to the exact one. It also indicates that the positron-electron cusp values would give indications of the accuracy for annihilation rate calculations.

In addition to the lifetimes and annihilation rates, another experimentally interesting parameter for the positronium negative ion is the two-photon angular correlation function $P(\theta)$. In most of the angular correlation measurements only one component of the momentum distribution is measured. The angle between the two photons, measured in the laboratory frame, has a value of $\pi - \theta$. The relation between θ and q_3 , the third component of the momentum, is $q_3 = mc\theta$, or $\theta = 7.3 \times 10^{-3} q_3$. The one-dimensional angular correlation function will have a form

$$P(q_3) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dq_1 dp_2 S(q) \quad (7)$$

where

$$S(\bar{q}) = \left| \int d\bar{r}_{1p} \exp(-i\bar{q} \cdot \bar{r}_{1p}) \Psi(\bar{r}_{1p}, \bar{r}_{2p}, \bar{r}_{12}) \right|_{\substack{r_{12} = r_{1p} \\ r_{2p} = 0}}^2. \quad (8)$$

The angular correlations functions were calculated in Ref. 11. The full width at the half maximum, denoted by 2Δ , was $1.3994 \times 10^{-3} \text{ rad}$. The smaller width of the angular correlation function for Ps^- is due to the following. Since the Ps^- ion is a loosely bound system, the momentum distribution of the Ps atom in Ps^- is smaller than the more tightly bound atomic counterparts. The angular correlation function for Ps^- is hence smaller. Furthermore, when the positron annihilates with one of the electrons in Ps^- to become two photons, a portion of the momentum of the two photons will be absorbed by the remaining electron because the mass of the electron is small.

We also reported a calculation on the two-photon-annihilation rates for the doubly excited resonant states in Ref. 20. The resonance positions were calculated by using the stabilization method.²¹ A positronium negative ion in its ground state will, of course, eventually undergo the annihilation process. The annihilation of positrons in a doubly excited state of Ps^- presents an interesting question. The autoionization process is now also possible, as is the radiative cascade to a lower autoionizing state or to the ground state. The radiative lifetimes are related to the oscillator strengths for transitions between the upper and lower states. They are usually small for low Z systems. The lifetimes of these various processes are of obvious interest, since such information would play an important role for experimental observations of the doubly excited states.

Calculations of annihilation rates for doubly excited states in Ps^- were done in Ref. 20. Results are summarized here in Table 3. The autoionization lifetimes were obtained by using the method of complex-coordinate rotation.²²

Table 3. Autoionization lifetimes and annihilation lifetimes for $1S^e$ doubly excited states of Ps^- .

| State | Autoionization lifetimes (nsec) | Annihilation lifetimes (nsec) | Annihilation rate (nsec^{-1}) |
|-------|---------------------------------|-------------------------------|--|
| 2s2s | 0.0005625 | 5.0277 | 0.1989 |
| 2s3s | 0.002419 | 6.9204 | 0.1445 |
| 3s3s | 0.0003225 | 23.474 | 0.0426 |
| 3s4s | 0.0004398 | 32.895 | 0.0304 |
| 4s4s | 0.0002016 | 80.000 | 0.0125 |

It is seen that for all the resonant states the system will have a greater probability to autoionize than to annihilate. Furthermore, when the quantum numbers of the outer electrons are the same, the annihilation rates decrease as $1/n^3$, as n represents the quantum numbers of the inner electrons. For example, the ratio of the annihilation rates for the 2s3s and 3s3s $1S^e$ states is $0.1445/0.0426 = 3.392$. The ratio of $(\frac{1}{2})^3/(\frac{1}{3})^3$ is 3.375. Similarly, the ratio of the annihilation rates for the 3s4s and 4s4s $1S^e$ states is $0.0304/0.0125 = 2.43$. The ratio of $(\frac{1}{3})^3/(\frac{1}{4})^3$ is 2.37. These results indicate that the annihilation of the positron in a doubly excited Ps^- takes place mostly with the inner electron since the overlap of the positronium S states also decreases as $1/n^3$. The findings in Ref. 20 were consistent with the earlier studies of the ground state of Ps^- that the positronium negative ion is a system of an electron loosely bound to a positronium atom.²³

Autoionizing resonance states in Ps^- are very similar to those of H^- . They are both the result of dipole degeneracy of the excited states of target systems. The first theoretical study²⁴ of doubly excited resonance phenomena in Ps^- were carried out by using the method of complex coordinate rotation.²⁵ Several resonances associated with the $N = 2$ and $N = 3$ Ps thresholds were reported. Since then, resonances associated with the $N = 5$ Ps threshold have been calculated.²⁶ They are now summarized in Table 4.

In addition to the calculations of the S-wave doubly excited states using the method of complex coordinate rotation, other methods have also been used to study resonance phenomena in Ps^- . For states with $L > 0$, results are summarized in Table 5. They were obtained by using the hyperspherical coordinates²⁷ and by scattering calculations.²⁸ However, in the hyperspherical coordinate, no widths were calculated. Also, in Ref. 28, a resonance structure was obtained in the $1P^o$ scattering calculation. None of the doubly excited resonant states has however been observed experimentally.

Table 4. Doubly excited resonances of Ps^- associated with positronium excitation threshold N . Resonance energies and widths are expressed in Rydbergs.

| N | $1S^e$ | | | | $3S^e$ | | |
|---|--------|-----------|----------|--|--------|---------|----------|
| | state | $-E_r$ | Γ | | state | $-E_r$ | Γ |
| 2 | 2s2s | 0.1520608 | 0.000086 | | 2s3s | 0.12706 | 0.00001 |
| | 2s3s | 0.12730 | 0.00002 | | | | |
| 3 | 3s3s | 0.070683 | 0.00015 | | 3s4s | 0.05873 | 0.00002 |
| | 3s4s | 0.05969 | 0.00011 | | | | |
| 4 | 4s4s | 0.04045 | 0.00024 | | 4s5s | 0.03415 | 0.00002 |
| | 4p4p | 0.0350 | 0.0003 | | | | |
| | 4s5s | 0.03463 | 0.00034 | | | | |
| 5 | 5s5s | 0.0258 | 0.00045 | | | | |
| | 5p5p | 0.02343 | 0.00014 | | | | |

Table 5. Doubly excited autoionizing states (with $L > 0$) of Ps^- below the $N = 2$ Ps threshold.

| | Botero (1988) ²⁷ | Ward, Humberston, and McDowell (1987) ²⁸ | |
|-----------|--------------------------------|--|---------------------|
| | (Hyperspherical coordinate) | (scattering calculation) | |
| | E(Ry) | E(Ry) | $\Gamma(\text{eV})$ |
| $3P^o(1)$ | -0.1456 | -0.14662 | 0.0035 |
| (2) | | -0.12509 | 0.001 |
| $1D^e$ | -0.13486 | | |
| $1P^o$ | -0.125174 | | |

Figure 2 shows the current understanding of the energy levels for Ps^- . I should also point out that very recently, a resonance lying just above the Ps ($N = 1$) threshold was predicted by Melezhik and Vakajlovic.²⁹ However, Bhatia and Drachman³⁰ reported in this workshop that they did not find such a resonance. It seems the existence for this resonance has yet to be established.

One implication from the current understanding of doubly excited Ps^- states as shown in Fig. 2 is that more studies on highly excited (associated with high N of Ps thresholds) are called for. In atomic physics one of the latest theoretical discoveries is the underlying symmetry of the doubly excited resonances in H^- and in helium. The striking similarity between the doubly excited spectrum of a two-electron atom and that of a linear triatomic molecule (XYX) has been investigated by Kellman and Herrick.³¹ In positronium negative ions, the study of the doubly excited resonances has just begun. Whether such highly symmetrical spectra will also be found in Ps^- is an open and interesting question.

It seems that a positronium ion does not have a $^3P^e$ state below the $\text{Ps}(N = 2)$ threshold, in contrast to the counterpart of H^- . Here, I am not going to talk about these studies in detail. Interested readers are referred to the original papers^{10,32,33} and the recent reviews. Other theoretical studies on Ps^- include calculations of photodetachment cross sections.^{34,35}

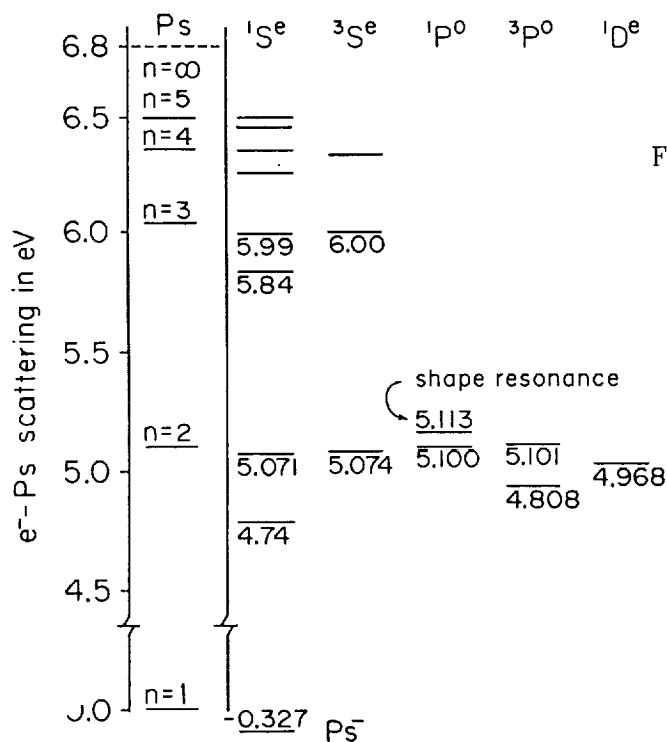


Fig. 2. Bound state and autoionizing states of Ps^- .

POSITRONIUM MOLECULES

Positronium molecules, Ps_2 , is a system consisting of two positronium atoms (or a four-particle system consisting of two electrons and two positrons, and interacted via Coulomb forces). The first calculation that showed such a system does form a bound system was by Hylleraas and Ore.³⁶ They showed that the binding energy for Ps_2 is 0.116 eV. Over the years, several theoretical studies have appeared in the literature for this system.³⁶⁻⁴¹ Results are summarized in Table 6. Possible experimental studies of positronium molecules have been discussed by Mills.⁴²

Table 6. Calculations of binding energies of positronium molecules.

| Authors | Binding energy | |
|---|---------------------|-------------------|
| | (Ry) | (eV) |
| Hylleraas and Ore 1947 (Ref. 36) | 0.0085 | 0.116 |
| Ore 1947 (Ref. 37) | 0.009 | 0.122 |
| Akimoto and Hanamura 1972 (Ref. 38) | 0.0135 | 0.184 |
| Brinkman, Rice, and Bell 1973 (Ref. 39) | 0.0145 | 0.197 |
| Lee, Vashista, and Kalia 1983 (Ref. 40) | 0.03 ± 0.002 | 0.408 ± 0.027 |
| Lee 1985 (Ref. 40) | 0.0303 ± 0.0005 | 0.412 ± 0.007 |
| Ho 1986 (Ref. 41) | 0.0302 | 0.411 |

A variational calculation was carried out by myself.⁴¹ I now discuss the work in the following. The Hamiltonian for this system was expressed as

$$H = \sum_{(i < j)} \left[-\left(\frac{1}{m_i} + \frac{1}{m_j} \right) \left(\frac{\partial^2}{\partial r_{ij}^2} + \frac{2}{r_{ij}} \frac{\partial}{\partial r_{ij}} \right) + \frac{2Z_i Z_j}{r_{ij}} \right] - \sum_{\substack{(i \neq j, k) \\ (j < k)}} \frac{2}{m_i} \cos(\theta_{ij,ik}) \frac{\partial^2}{\partial r_{ij} \partial r_{ik}}, \quad (9)$$

with

$$\cos(\theta_{ij,ik}) = \frac{r_{ij}^2 + r_{ik}^2 - r_{jk}^2}{2r_{ij}r_{ik}}$$

where m_i and Z_i are the mass and charge of the particle i , respectively. Atomic units were used with energy expressed in Rydbergs. Figure 3 shows the coordinate system where a and b denote the positrons, and 1 and 2 the electrons. The interparticle coordinate r_{1a} represents the distance between the electron 1 and the positron a .

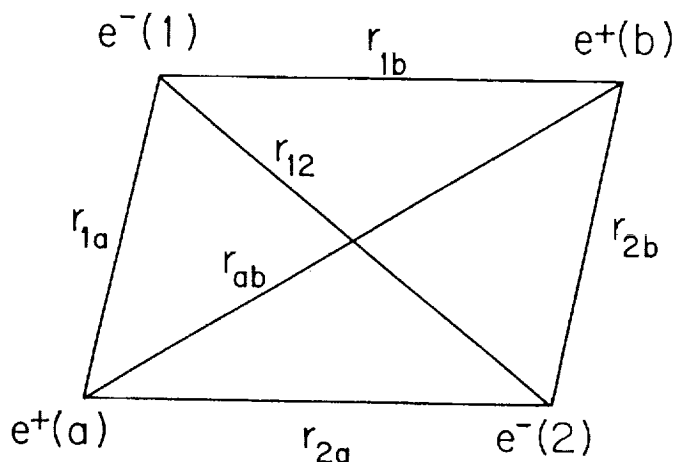


Fig. 3. Coordinate system for Ps_2 .

A general form of wave function for positronium molecules is

$$\begin{aligned}
\Psi = & \sum C_{kmnijl} \left[r_{1a}^k r_{2a}^m r_{ab}^n r_{2b}^i r_{1b}^j r_{12}^l \exp(-c_1 r_{1a} - c_2 r_{2a} - c_3 r_{ab} - c_4 r_{2b} - c_5 r_{1b} - c_6 r_{12}) \right. \\
& + r_{1a}^m r_{2a}^k r_{ab}^n r_{2b}^j r_{1b}^i r_{12}^l \exp(-c_2 r_{1a} - c_1 r_{2a} - c_3 r_{ab} - c_5 r_{2b} - c_4 r_{1b} - c_6 r_{12}) \\
& + r_{1b}^k r_{2b}^m r_{ab}^n r_{2a}^i r_{1a}^j r_{12}^l \exp(-c_1 r_{1b} - c_2 r_{2b} - c_3 r_{ab} - c_4 r_{2a} - c_5 r_{1a} - c_6 r_{12}) \\
& \left. + r_{1b}^m r_{2b}^k r_{ab}^n r_{2a}^j r_{1a}^i r_{12}^l \exp(-c_2 r_{1b} - c_1 r_{2b} - c_3 r_{ab} - c_5 r_{2a} - c_4 r_{1a} - c_6 r_{12}) \right] \\
& \times \frac{1}{\sqrt{2}} (\alpha_1 \beta_2 - \beta_1 \alpha_2) \frac{1}{\sqrt{2}} (\alpha_a \beta_b - \beta_a \alpha_b), \tag{10}
\end{aligned}$$

where α and β are the spin-up and -down wave functions, respectively. The wave function in the form of Eq. (2) is antisymmetric with respect to interchange of the two electrons or of the two positrons. To solve the necessary integrals involved in this extensive form of wave functions is not an easy task. Some simplifications were hence made in Ref. 41. First, we omitted the symmetry of the two positrons, i.e., the last two terms in Eq. (2) were dropped. Secondly, we let $C_4 = C_5 = C_6 = 0$. The omission of the explicit exponential factors involving r_{1p} , r_{2p} , and r_{12} will be compensated by the use of extensive terms involving power series of such interparticle coordinates. Under these approximations, the wave function becomes

$$\begin{aligned}
\Psi = & \sum C_{kmnijl} \left[r_{1a}^k r_{2a}^m r_{ab}^n r_{2b}^i r_{1b}^j r_{12}^l \exp(-c_1 r_{1a} - c_2 r_{2a} - c_3 r_{ab}) \right. \\
& \left. + r_{1a}^m r_{2a}^k r_{ab}^n r_{2b}^j r_{1b}^i r_{12}^l \exp(-c_1 r_{2a} - c_2 r_{1a} - c_3 r_{ab}) \right] \\
& \times \frac{1}{\sqrt{2}} (\alpha_1 \beta_2 - \beta_1 \alpha_2). \tag{11}
\end{aligned}$$

Up to $N = 400$ terms were used in Ref. 41. The ground state energy is shown here in Table 7, together with cusp values for different pairs of charged particles. It is seen that the cusp values are quite close to the exact ones. Table 6 lists different calculations of binding energy of Ps_2 in the literature. Ref. 41 is a variational bound calculation and the result in Ref. 40 was obtained by using the Green's Function Monte Carlo method. This method, however, is not a bound calculation and has statistical errors. I should also point out that calculations of binding energy with considerable larger values (0.978 eV and 0.846 eV) also exist in the literature.^{43,44} It appears that these calculations should be repeated. As for the variational calculation in Ref. 41, although the binding energy is reliable, the book is by no means closed. For example, wave functions that take into account of the proper symmetry for the two positrons should be used (i.e., Eq. 10) in the future.

Table 7. Energy and cusp values for positronium molecules:
 $\omega = k + m + n + i + j$, with $m = 0$ (see Ref. 41)

| | E (Ry) | ν_{1a} | ν_{12} | ν_{ab} | ν_{1b} |
|------------------------------------|----------|------------|------------|------------|------------|
| $\omega = 6, \ell \leq 4, N = 400$ | -1.03021 | -0.498 | 0.485 | 0.509 | -0.479 |
| Exact | | -0.5 | 0.5 | 0.5 | -0.5 |

Table 8 shows the average distances between various pairs of charged particles. One of the interesting results shown in Table 8 is that all the six interparticle distances seem to have the same value of $5.9a_0$ (if we assign a 10% uncertainty to $\langle r_{1b} \rangle$). This suggests that on average, the four particles form a triangular pyramid, with the two electrons occupying any two of the four vertices, and the two positrons occupying the other two. All the six edges have the same length of $5.9a_0$. In this arrangement, the system is symmetric with respect to the interchange of the two electrons, or of the two positrons, as well as to the interchange of the two positronium atoms.

Table 8. Average distances (in a_0) between various pairs of charged particles
(see Ref. 41)

| $\langle r_{1a} \rangle = \langle r_{2a} \rangle$ | $\langle r_{12} \rangle$ | $\langle r_{ab} \rangle$ | $\langle r_{1b} \rangle = \langle r_{2b} \rangle$ |
|---|--------------------------|--------------------------|---|
| 5.98 | 5.93 | 5.88 | 5.50 |

We have also recently begun a theoretical study of higher-lying resonant states of positronium molecules.^{45,46} In some aspects, these high-lying states are similar to those in a positronium hydride, PsH . In PsH , it has been shown that Rydberg series do exist as a result of the positron attaching to the H^- ion.⁴⁷ Such Rydberg states, with the exception of the lowest S-wave state which lies below the $Ps + H$ threshold and becomes the ground state of PsH , would appear as resonances in $Ps - H$ scattering. We would, therefore, expect such Rydberg series to also exist in the Ps_2 molecules as a result of the positron attaching to Ps^- ions. Figure 4 shows the Coulomb potential between the positronium negative ion and the positron, and the resulting Rydberg series. The lowest state of the S-wave series also lies below the $Ps - Ps$ scattering threshold and becomes the ground state of the positronium molecules.⁴¹ Higher members of the Rydberg states would lie in the $Ps - Ps$ scattering continuum and appear as resonances in $Ps - Ps$ scattering.

There is, however, a difference between resonances in $Ps - H$ scattering and $Ps - Ps$ scattering. In the latter case there are two Rydberg series since the total spin of the two positrons would form singlet or triplet spin state. In the former case there is one series for a given partial wave since the positron and proton are not identical. We located six members of resonances below the Ps^- threshold. Results are summarized in Table 9. It was suggested that three of them belong to a Rydberg series in which the two positrons form a singlet spin state and the other three members belong to a series in which the two positrons form a triplet spin state. In the former case the complex eigenvalues would appear as resonances in scattering between two orthopositronium (o-Ps) atoms or two parapositronium (p-Ps) atoms. In the latter case, the complex eigenvalues correspond to resonances between a p-Ps atom and an o-Ps atom. Figure 5 shows the resonance positions for these autodissociating states. It should be mentioned that the

classification of different spin states for the resonances in Table 9 is just tentative. For the wave functions we used in Ref. 46, it was not straightforward to identify the positron spin state to which a resonance belongs. Interestingly enough, the use of wave functions of Eq. (11) enabled us to obtain resonance parameters for the two series with different spin symmetries simultaneously.

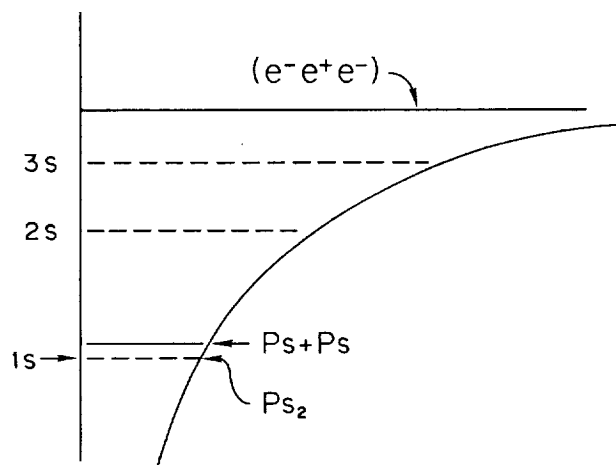


Fig. 4. Coulomb potential and Rydberg states between a positron and a positronium ion. Ignore the spins of the positrons for the time being.

Table 9. Autodissociating resonant states in Ps_2 . (see Ref. 46)

| Resonant state | $E(\text{Ry})$ | $\Gamma(\text{Ry})$ | $E(\text{eV})^a$ | $\Gamma(\text{eV})$ |
|----------------|----------------------|---------------------|------------------|---------------------|
| Triplet series | | | | |
| 2S | -0.6588 | 0.0056 | 4.642 | 0.0762 |
| 3S | -0.592 | 0.0080 | 5.551 | 0.109 |
| 4S | -0.5625 | 0.0030 | 5.946 | 0.041 |
| Series limit | -0.5240 ^b | | 6.476 | |
| Singlet series | | | | |
| 2S | -0.626 | 0.016 | 5.089 | 0.216 |
| 3S | -0.580 | 0.012 | 5.714 | 0.163 |
| 4S | -0.553 | 0.016 | 6.082 | 0.216 |
| Series limit | -0.5240 ^b | | 6.476 | |

^aRelative to $Ps - Ps$ scattering threshold.

^bSee Ref. 11 for example.

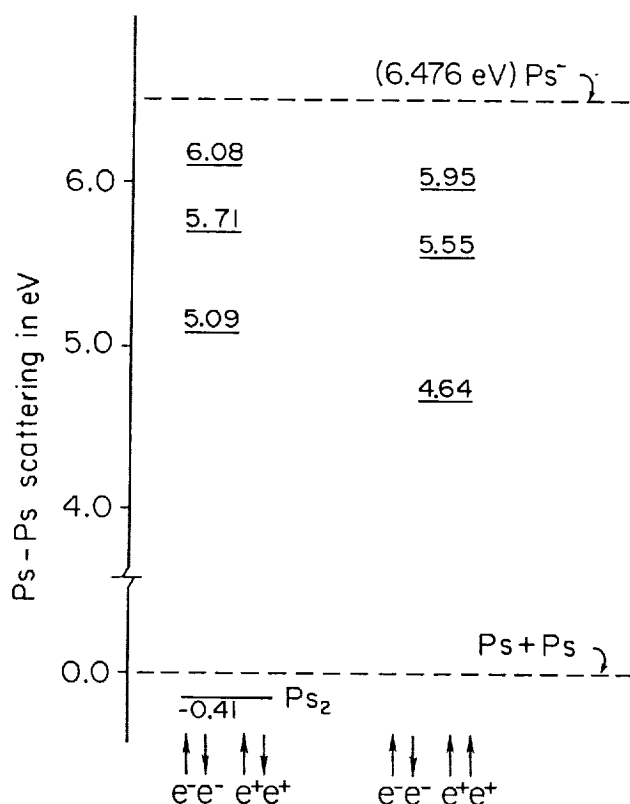


Fig. 5. Bound state and autoionizing states in Ps_2 .

CONCLUDING REMARKS

In this talk, I have discussed the recent advances of theoretical studies for two atomic systems involving positrons. In closing, let me speculate what might happen in future workshops. Ever since the discovery of positrons, increasingly complicated atomic systems involving positrons have been studied. Various properties for positronium atoms (1 electron, 1 positron) and positronium ions (2 electron, 1 positron) were studied both experimentally and theoretically. The next complicated system is positronium molecules (2 electrons, 2 positrons), Ps_2 . As I have mentioned in this talk that theoretical studies on this system have a long history, the observation for such species has yet to be done. The next complicated system would be "positronium molecular ions" (3 electrons, 2 positrons), Ps_2^- . Of course, we don't even know this five-body system would form a stable bound state. But in any case, the dissociative attachment process ($e^- + \text{Ps}_2 \rightarrow \text{Ps} + \text{Ps}^-$) would be of interest. Next, if we add one more positron to this system, this six-particle system (3 electrons, 3 positrons) may form a tri-atomic positronium molecule, Ps_3 . Again, whether they would form a stable system is an interesting question. Furthermore, if we extend our imagination, we would ask what happens to a system consisting of n positronium atoms (n electrons, n positrons). Would they form positronium clusters? Perhaps in future positron workshops, some of these questions about such exotic species would be answered.

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